Fractal Character of Eigenstates in Disordered Systems

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Electronic eigenfunctions are studied on the tight-binding model of disordered systems at dimensionalities $d=1,2,3$. It is found that the eigenfunctions have a self-similar (fractal) behavior up to length scales roughly equal to the localization length. For $d=3$, above the mobility edge, the fractal character persists up to length scales about equal to the correlation length ξ. The dependence of the fractal dimensionality D on disorder W is presented. The fractal character of the wave function is suggested as a *new method* for finding mobility edges.

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There has always been a problem of how to characterize the quantum eigenfunctions of the disordered systems. One characterization is the localization length λ, which describes the exponential decay of the localized states. Another is the correlation length ξ which describes the spatial extent of the amplitude fluctuations of extended states. As a result of recent interest in studying the fractal (self-similar) character of clusters in percolating models,[1-4] it is important to test whether the electronic eigenfunctions in disordered systems are also fractal.

Before discussing our new results let us briefly review the results from percolation theory, which motivated this study. It is now well known that for the *classical* percolation, it has been demonstrated[2,3] that a percolation correlation length ξ_p exists, which diverges as $\xi_p \sim |p-p_c|^{-\nu}$ at the critical concentration p_c. For lengths L much larger than ξ_p the system looks homogeneous. However, both Monte Carlo simulations[2,3] and experiments[4] show that the clusters are not homogeneous for length scales L which are in the range $a \leq L \leq \xi_p$ (a is the interatomic distance). In this range, the clusters are self-similar and the number of links (or sites) which belong to a given cluster within a volume L^d (in d dimensions) varies as L^D, with the fractal dimensionality[1,2] $D=d-\beta'/\nu$. Here β' and ν are the density and correlation-length exponents, respectively. Note that this property is expected for both *finite* and infinite clusters. For the classical percolation case it has been shown experimentally[4] that $D=1.90\pm0.02$ for $d=2$ independent of the concentration p of the conducting links.

In this Letter we systematically examine the fractal character of the wave functions[5] in $d=1$, 2, and 3 dimensions for disordered systems. The fractal dimensionality D is obtained and its dependence on the disorder is examined.

There is ample evidence from numerical work[6,7] in one-dimensional (1D) and 2D disordered systems and from analytical studies in 1D systems[8] that the localized eigenfunctions fluctuate widely (in addition to their exponential decay), having thus a fragmented character. Even the extended states for 3D systems above the mobility edge are expected to show strong amplitude fluctuations up to a length ξ; for length scales above ξ the extended states look uniform. The existence of the length ξ is a consequence of the scaling theory of localization.[9-14] The latter is based upon the assumption that there is a single scaling variable, the dimensionless conductance $g(L)$, which determines the localization properties of a physical system. It is further assumed that the quantity $\beta=d\ln g/d\ln L$ is a monotonic and nonsingular function of g.

The fragmented character of the eigenfunctions strongly suggests that they may be fractal objects. Mandelbrot[15] has pointed out that the fractal dimensionality of such an object embedded in d-dimensional space can be determined from the relation $\int_0^L dr\, r^{d-1}\rho(\vec{r}) \sim L^D$, where $\rho(\vec{r})$ is the density. Unfortunately this relation is not applicable to a strongly random system because of the strong dependence of the integral on the origin. One way to avoid this difficulty is by averaging over all possible choices of origin, each weighted by the density (or probability) itself:

$$A(L) \equiv \int d^d r_0 \rho(\vec{r}_0) \int_0^L dr\, r^{d-1} \rho(\vec{r}+\vec{r}_0) = c\, L^D, \quad (1)$$

where c is a constant. Our numerical study reported below showed that Eq. (1) is well satisfied (for $a \lesssim L \lesssim \xi, \lambda$, where λ is the localization length). Thus we were in a position to determine for the first time the fractal dimensionality of the eigenfunctions in a disordered quantum system. This allowed us to check the recent suggestion by Cohen, Economou, and Soukoulis[16] that $D=2$

$+\beta$, for $\beta > 0$.

We consider a tight-binding model defined by the Hamiltonian

$$H = \sum_n \epsilon_n |n\rangle\langle n| + \sum_{n,m} V_{nm} |n\rangle\langle m| , \qquad (2)$$

where ϵ_n are random variables given from a rectangular probability distribution of width W. In the present study the system has no off-diagonal disorder, i.e., V_{nm} is nonzero and equal to V (which is taken as the unit of energy) only when n and m are nearest neighbors.

We have numerically calculated the wave functions for $N = 5000$ sites in 1D, $N = 50 \times 50$ sites in 2D, and $N = 16 \times 16 \times 16$ sites in 3D. We also impose periodic boundary conditions. We have calculated several (five in this work) eigenfunctions corresponding to eigenvalues close to any given energy E. A calculated eigenfunction defined as $H\psi = E\psi$ is expressed as $\psi = \sum_i c_i |i\rangle$ for each eigenvalue E. We normalize the eigenfunctions so that $\sum_i |c_i|^2 = 1$; then $\rho(\vec{r}_i) \equiv \rho_i \equiv |c_i|^2$ and the fractal dimensionality is determined[17] by the discretized version of Eq. (1).

Note that for a uniform normalized wave function $\rho(\vec{r}) = \text{const}$ and $\int d^d r\, \rho(\vec{r}) = 1$; therefore $A(L) = L^d$. Our results for the three different dimensions are as follows:

1D case.—It is by now well established that in a 1D model all eigenstates are localized regardless of the amount of disorder. There exists a length scale, the localization length λ, above which one sees the exponential decay of the wave function. For lengths up to localization length λ the wave function has a fractal character as one can see from Fig. 1(a) where we plot $\ln A(L)$ vs $\ln L$ for different amounts of disorder for $E = 0$. As expected $\ln A(L)$ vs $\ln L$ follows a straight line rather well and then bends over. The point of bending is expected to be correlated with the localization length. However, because there are substantial fluctuations in the behavior of eigenfunctions belonging to the same energy and the same disorder W, the point of bending fluctuates appreciably from eigenfunction to eigenfunction and hence it may be significantly different from the localization length which is denoted by an arrow in our figures. Note that for low disorder the fractal dimensionality is close to 1 and decreases as disorder increases. For a given disorder we have generated five different eigenstates and for each of them we plot $\ln A(L)$ vs $\ln L$. By least-squares fitting we get the slope which is the fractal dimensionality D. Then we average D over the five eigenfunctions. This procedure has been done by the computer to eliminate any bias errors by us. In Fig. 1(b) we plot the average value of D as a function of disorder for $E = 0$. Note that D decreases as disorder increases. At the same time λ decreases, and therefore the length scale over which the fractal character of the wave function is obeyed decreases.

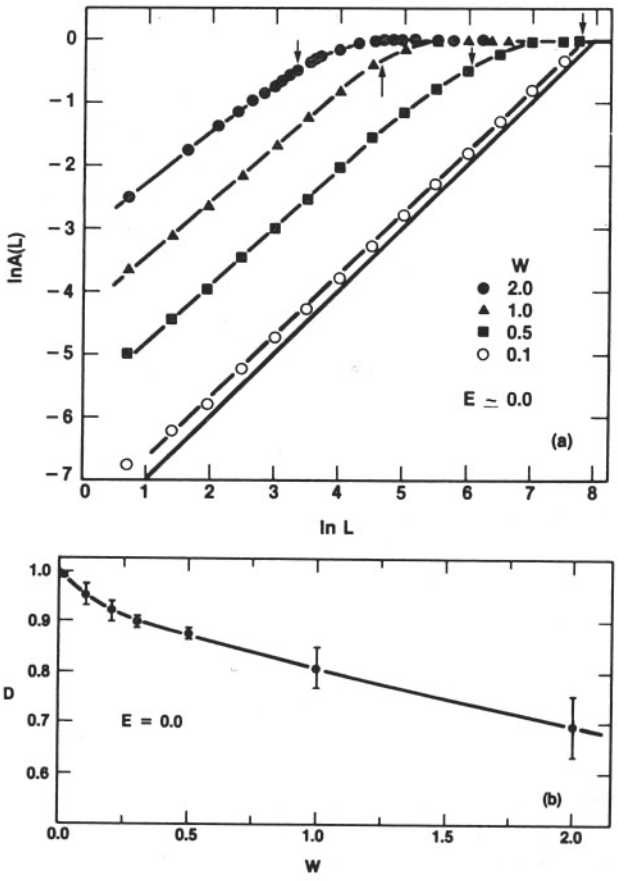

FIG. 1. (a) Plot of $\ln A(L)$ vs $\ln L$ for different amounts of disorder W at the center of the band $E = 0$ for a 1D disordered system. The arrows denote the value of the localization length. The solid line has slope 1, the value for extended states. (b) Fractal dimensionality D of the eigenstates vs disorder W for 1D disordered system at the center of the band. Error bars come from averaging D over five random configurations.

2D case.—Our results for the 2D case are similar to those of the 1D case. For length scales $L \lesssim \lambda$ the wave function is self-similar down to almost interatomic distances. This is clearly seen in Fig. 2(a) where we plot $\ln A(L)$ vs $\ln(2L+1)$ for different disorders W for $E = 0.45$. As in the 1D case we have calculated the fractal dimensionality D for five eigenstates with eigenvalues[18]

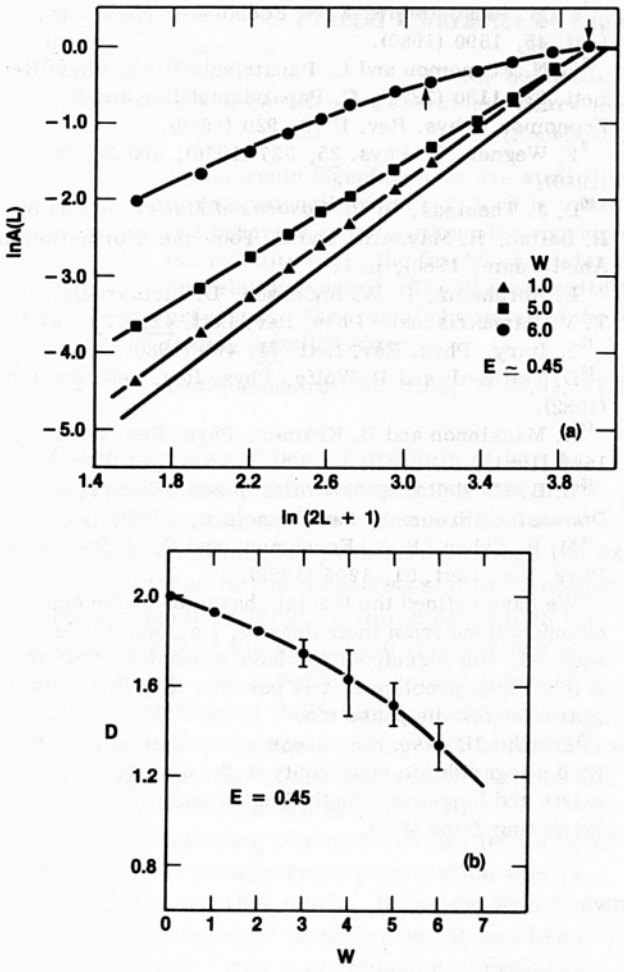

FIG. 2. (a) Plot of $\ln A(L)$ vs $\ln(2L+1)$ for different amounts of disorder W at $E=0.45$ for a 2D disordered system. The arrows denote the value of the localization length. The solid line has slope 2, the value for extended states. (b) Fractal dimensionality D of the eigenstates vs disorder W for a 2D disordered system at $E=0.45$. Error bars come from averaging D over five random configurations.

around $E=0.45$ and plot it as a function of disorder. Note that as disorder increases, D decreases. Of course as W increases, λ decreases and therefore the self-similar region diminishes.

3D case.—The 3D case is the most interesting one because a mobility edge exists. At the mobility edge there is no upper length scale (both λ and ξ blow up there) and the fractal character continues at all lengths. On the other hand, the size of the system that we can treat numerically, although no less than in previous numerical studies, is still not big enough to allow definite conclusions.

The expected behavior is as follows: For disorder not enough to produce localization and for length scales larger than a but less than ξ, $\ln A$ vs $\ln(2L+1)$ must have a slope $D<3$. Well above ξ the slope must increase to 3. At the mobility edge the slope D must be a constant less than 3 at all length scales. Finally for strong disorder, when states are localized, a constant slope $D<3$ will be maintained up to a distance roughly equal to the localization length λ; well above λ, $\ln A$ vs $\ln(2L+1)$ is expected to bend over and show a saturation behavior.

Such a behavior was found for the $E\simeq 0$ states of a 3D system. We studied several values of W. For each value of disorder we calculated five different eigenfunctions each of eigenenergy very close to zero. Because of the relatively small size of our sample, the plot of $\ln A$ vs $\ln(2L+1)$ did not in general follow a straight line as well as was found for $d=1$ and 2. The slope as determined from a least-squares fit fluctuated significantly from eigenfunction to eigenfunction. As a result there is a rather large uncertainty in our values of D. We find $D=1.9\pm0.3$, 1.7 ± 0.3, and 1.3 ± 0.3 for $W=14$, 16, and 20, respectively. To estimate fractal dimensionality D_c at the mobility edge we must know the critical value, W_c, of W. It was recently estimated[14] that $W_c\approx 16$. Our present preliminary results suggest that $W_c\approx 17\pm2$. Thus our estimate for D_c is $D_c\approx 1.7\pm0.3$. This value seems to be in clear disagreement with the first-term-in-ϵ (where $\epsilon=d-2$) result for D_c obtained by Wegner[9] ($D_c=2-\epsilon$), while it is reasonably close to the value $D_c=2$ suggested by Cohen, Economou, and Soukoulis.[16]

It is worthwhile to point out that a by-product of the present study is a new method for obtaining the critical disorder $W_c(E)$ for localization. The plot of $\ln A(L)$ vs $\ln(2L+1)$ bends upwards for $W<W_c$, is a straight line for all lengths at $W=W_c$, and bends downwards for $W>W_c$. The method determines W_c to be within the limits $W_1<W_c<W_2$, where $\xi(W_1)\simeq L_{\max}$ and $\lambda(W_2)\simeq L_{\max}$; $L_{\max}$ is the maximum size of the random system for which one can numerically obtain the eigenstates. An alternative may be to obtain W_c by numerically solving the equation $D(W_c)=D_c$, where D_c is the fractal dimensionality at the mobility edge. Of course, an improved estimate of D_c is needed.

In conclusion, we have numerically demonstrated for the first time that for $a<L<\min(\xi,\lambda)$ the eigenfunctions in disordered systems have a fractal character. Thus the amplitude of the eigenfunctions is characterized quantitatively not

only by a length scale ξ or λ but by a fractal dimensionality D as well. We have also obtained explicit numerical results for the dependence of D on the disorder.

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[17]We have defined the fractal character of the quantum eigenfunctions from their density, i.e., amplitude squared. But eigenfunctions have a phase as well and it is an open problem if it is possible to define a fractal character for the phase too.

[18]For the 2D case, we choose $E \neq 0$ since at $E = 0$ for $W = 0$ a logarithmic singularity in the density of states exists and long-wavelength fluctuations prevent us from extracting D for $W = 0$.